

Solid-phase epitaxial growth of (111)-oriented Si film on $\text{InGaO}_3(\text{ZnO})_5$ buffer layer

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Abstract In this paper, the (0001) surface of an $\text{InGaO}_3(\text{ZnO})_5$ (c-IGZO) single-crystal buffer layer was used as a seed layer to control the orientation of a Si film in solid-phase heteroepitaxial growth at 950 °C. Despite a large lattice misfit of 20%, electron backscattering diffraction (EBSD) and transmission electron microscope (TEM) measurements substantiated that the (111)-oriented Si layers are grown epitaxially on the c-IGZO (0001) surface, which is explained by domain-matched epitaxy. The process can be further developed for low temperature process by utilizing excimer laser annealing to produce highly uniform (111) oriented Si TFT over a large area.

1 Introduction

Si epitaxially growth [1–3] has been widely used in today's IC technology. An important application is to

grow highly uniform oriented crystal Si to integrate display drivers and radio-frequency circuits on a glass substrate. However, the conventional Si epitaxial growth requires a single-crystal Si substrate as a seed layer, which makes the process very expensive or even impossible for large-area applications. Excimer laser annealing (ELA) is widely used to fabricate high-quality low temperature polycrystalline Si (LTPS) without a damage to a glass substrate [4–6]. Amorphous silicon (a-Si) melts during laser pulse irradiation and solidifies during epitaxial growth [7]. However, due to lack of a seed substrate, the crystallites orientation of polycrystalline Si grown on glass is random because nucleation and growth of individual grains occur independently without orientation coherence between the crystallites. Metal-induced-crystallization (MIC) by e.g. Ni [8–10] and Al [11–14] can crystallize an a-Si layer at a low temperature with an orientation preference. However, the MIC approach produces epitaxial layers heavily contaminated with metal-related impurities (>0.1%). Moreover, grain boundaries and intra-grain defects limit the film quality and the carrier transport properties. Thus, the challenge is to use a seed layer for Si epitaxial growth.

Conventional (111)-oriented solid-phase epitaxial growth [15–18] has been achieved by utilizing lattice-matched epitaxy during thin-film growth as long as the lattice misfit is less than 8%. On the other hand, Narayan et.al [19, 20] has showed that a large lattice misfit relative to the substrate can still grow epitaxial layers, which is called 'domain matching epitaxy (DME)', where integral multiples of the lattice constants make a good lattice matching between the substrate and the over-grown layer [21]. DME occurs preferably if the surfaces of the substrate and the film have similar crystal structures (i.e. similar atomic configurations) and the chemical bonds between the

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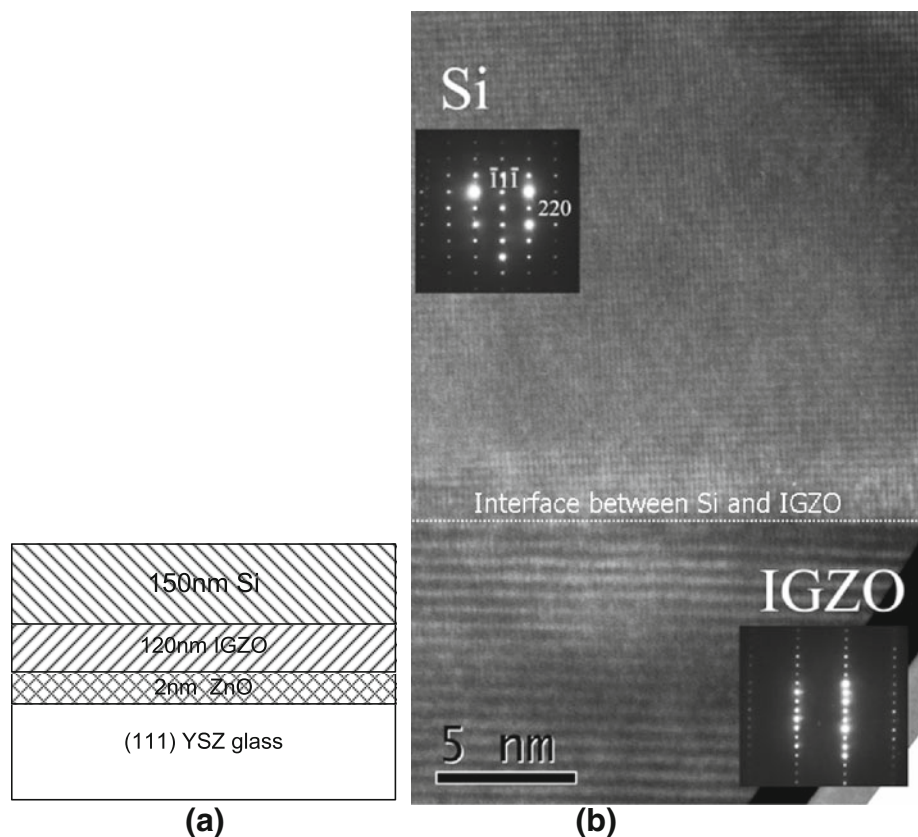
substrate and the film is not so strong, which is the case for e.g. ionic crystals such as oxides. Many systems with a large misfit have been grown by DME [22–26]. This gives possibility that Si can grow epitaxially on a substrate even with a large lattice misfit $>8\%$.

Oxide semiconductor materials with a wide band gap have attracted many interests. For instance, zinc oxide (ZnO) has been studied intensively because ZnO can produce operating semiconductor devices at a low temperature or even room temperature. Hosono et al. [27] reported that (0001) $\text{InGaO}_3(\text{ZnO})_5$ (IGZO) single-crystal films are grown epitaxially on a yttria-stabilized zirconia (YSZ) substrate. It is also reported that ZnO can easily be textured to (0001) even on a glass substrate [28, 29]. Although the lattice mismatch between Si and c-IGZO is larger than 20%, (111) oriented Si can still epitaxially grow on (0001) oriented c-IGZO by domain matching epitaxy (DME) [21]. (111) oriented Si surface has three-fold rotational symmetry. And the surface symmetry of (0001) oriented c-IGZO is trigonal with three-fold rotational symmetry that matches with that of the Si (111) plane. This makes IGZO to be a good candidate as a seed layer for (111) Si epitaxial growth for a low temperature process.

2 Experiment

Figure 1a shows the structure of the cross-section. In order to obtain the single-crystal IGZO films, pulsed laser deposition (PLD) was first used to deposit a 2 nm-thick ZnO epitaxial layer at a substrate temperature of 700 °C on a (111) oriented single-crystal yttrium-stabilized zirconium (YSZ) substrate as the template. Then, a 120 nm-thick amorphous InGaZnO_4 (a-IGZO) layer was deposited at room temperature. Then the IGZO film was deposited in a gas mixture of argon and oxygen. The deposition condition of IGZO film was as follows: The ratio of O_2 to Ar was 1:19. The RF power was 70 W. The total gas pressure during the deposition was 0.55 Pa. The resulting bilayer structure was covered with a YSZ plate to suppress the evaporation of the film components and heated up to 1,400 °C for 30 min in an atmospheric electric furnace, resulting in the growth of (0001)-oriented single crystal. After that, a 150 nm thick Si layer was deposited by physical vapor deposition (PVD) at 450 °C. Then the sample is further annealed at 950 °C [18] in an atmospheric electric furnace to crystallize the Si film. The temperature was same as a previous paper which reports (111) epitaxial growth of Si on Si seed substrate [18].

Fig. 1 Structure of cross section and TEM cross section of Si epitaxial growth on c-IGZO



3 Results and discussion

Figure 1b shows a cross-sectional TEM image of the sample. With a lattice misfit of $>20\%$ for Si epitaxy over c-IGZO(0001), it is beyond the critical strain (8%) of conventional lattice matching. However, epitaxial growth of Si on c-IGZO is demonstrated by the concept of domain matching epitaxy. The diffraction pattern indicated that (111)-oriented Si is grown epitaxially on (0001)-oriented c-IGZO.

A Philips XL50 SEM equipped with an EDAX-EDAX-TSL Crystal EBSD system was used for EBSD analyses. The EBSD measurements were performed at an accelerating voltage of 25 kV with the spot size of 6 nm. Pseudo-Kikuchi patterns were integrated for 0.03 s, and the step for orientation mapping was about $0.2\ \mu\text{m}$ step in each analysis point. The backscattered electrons from a Kikuchi pattern can be indexed to generate a unique description of the local orientation. The samples were tilted 75 during the EBSD measurements. Figure 2a shows an EBSD mapping of the surface orientation of the Si film on the c-IGZO in the area of $1.2 \times 1.5\ \mu\text{m}^2$. We see the film has (111) orientation and no grain-boundary is found inside. Figure 2b shows a 001 pole figure and an inverse pole of the Si film. In the pole figure we can see one group of (111)

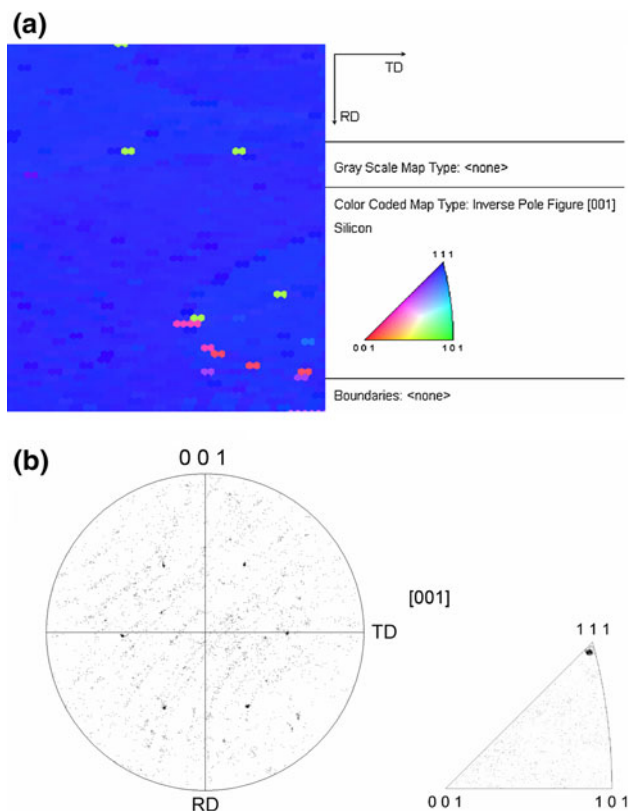


Fig. 2 Pole figure and inverse pole figure of Si by EBSD mapping

orientation, which means that the in-plane orientation control has also been achieved.

Figure 3 shows the crystal structure of the Si/c-IGZO sample. The InO_2^- layers and the $\text{GaO}(\text{ZnO})_5^+$ blocks are alternately stacked along the (0001) axis. The (111) oriented Si surface with $(1\bar{1}0)$ in-plane has a three-fold rotational symmetry ($a = 0.3829\ \text{nm}$). Moreover, the surface symmetry of (0001) oriented c-IGZO ($a = 0.3299\ \text{nm}$) is trigonal with a three-fold rotational symmetry. Epitaxial growth of Si (111) on c-IGZO (0001) occurs via matching 5 periods of Si and 6 periods of IGZO.

4 Conclusion

In conclusion, we successfully grew (111) single-crystal Si by solid-phase epitaxial growth on an $\text{InGaO}_3(\text{ZnO})_5$ layer by domain matching epitaxy (DME). By matching 6 planes of the Si with 7 planes of c-IGZO, it is possible to grow (111)-oriented crystal Si on (0001) c-IGZO substrate. The epitaxial temperature in this work is $950\ ^\circ\text{C}$, which can be decreased to room temperature by excimer laser annealing

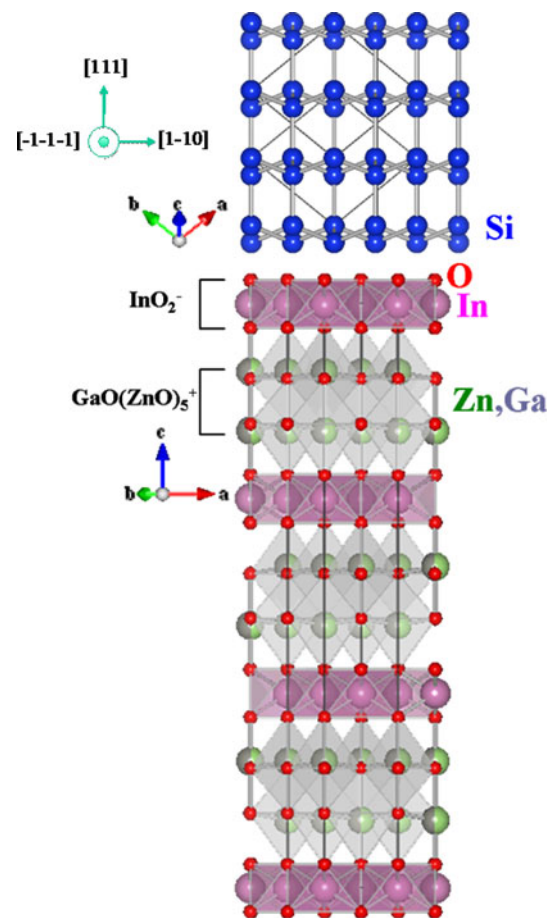


Fig. 3 Crystal structures of IGZO and Si

in the future. This process is very promising for producing (111) oriented crystal Si layer over large area on a glass substrate.

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